Malaoxon 1634-78-2 | DTXSID9020790

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Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 223 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.97e-01

Confidence level: 6.58e-01

Nearest Neighbors from the Training Set

Image not found

Malathion
Measured: 229
Predicted: 257

Image not found

Ethyl phthalyl ethyl glycolate

Measured: 347 Predicted: 319

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Crotoxyphos
Measured: 100
Predicted: 123

Image not found

Fenamiphos sulfone Measured: 43.7 Predicted: 56.5 Image not found

Thiophanate-methyl Measured: 1780 Predicted: 864